

INTERNATIONAL SEARCH REPORT

International Application No
PCT/US2004/035444

A. CLASSIFICATION OF SUBJECT MATTER
IPC 7 G01N23/207

According to International Patent Classification (IPC) or to both national classification and IPC

B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)
IPC 7 G01N

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practical, search terms used)
EPO-Internal, INSPEC

C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category *	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X	<p>A. LE BAIL: "Monte Carlo indexing with McMaille" STRUCTURE SOLUTION FROM POWDER DIFFRACTION DATA SSPD03, [Online] 14 September 2003 (2003-09-14), pages 1-31, XP002326866 CONGRESS CENTER ACADEMIA, STARA LESNA, SLOVAKIA Retrieved from the Internet: URL:http://sdpd.univ-lemans.fr/ppt/LeBail-SSPD03.ppt> [retrieved on 2005-04-28] page 9 entitled "What is examined in the automated 'black box' mode ?" page 11 entitled "'Simplicity' of the Monte Carlo algorithm in McMaille" -/--</p>	1-28,30,32,34,35

☒ Further documents are listed in the continuation of box C.

☐ Patent family members are listed in annex.

* Special categories of cited documents :

- "A" document defining the general state of the art which is not considered to be of particular relevance
- "E" earlier document but published on or after the international filing date
- "L" document which may throw doubts on priority claim(s) or which is cited to establish the publication date of another claim or other special reason (as specified)
- "O" document referring to an oral disclosure, use, exhibition or other means
- "P" document published prior to the international filing date but later than the priority date claimed

- "T" later document published after the international filing date or priority date and not in conflict with the application but cited to understand the principle or theory underlying the invention
- "X" document of particular relevance; the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone
- "Y" document of particular relevance; the claimed invention cannot be considered to involve an inventive step when the document is combined with one or more other such documents, such combination being obvious to a person skilled in the art
- "&" document member of the same patent family

Date of the actual completion of the international search

4 May 2005

Date of mailing of the international search report

22 07. 2005

Name and mailing address of the ISA

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C.(Continuation) DOCUMENTS CONSIDERED TO BE RELEVANT

Category *	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
L	-& ARMEL LE BAIL: "LISTE COMPLETE des PRODUCTIONS SCIENTIFIQUES 1976 - 2004"[Online] pages 13-13, XP002327153 Retrieved from the Internet: URL:http://pcb4122.univ-lemans.fr/rapport/LeBail_promo2004_prod.pdf> [retrieved on 2005-04-28] The reference to SSPD03 on page 13 and the associated link	1-28,30, 32,34,35
P,X	-& LE BAIL A: "Monte Carlo indexing with McMaille" POWDER DIFFRACTION AIP FOR JCPDS-INT. CENTRE FOR DIFFRACTION DATA USA, vol. 19, no. 3, September 2004 (2004-09), pages 249-254, XP009047070 ISSN: 0885-7156 abstract page 250, left-hand column, last paragraph - page 251, right-hand column, paragraph 2; table II page 254, chapter "IX. CONCLUSION" page 254, chapter "ACKNOWLEDGEMENT"	1-28,30, 32,34,35
X	COELHO A A: "Indexing of powder diffraction patterns by iterative use of singular value decomposition" JOURNAL OF APPLIED CRYSTALLOGRAPHY MUNKSGAARD INTERNATIONAL BOOKSELLERS & PUBLISHERS DENMARK, vol. 36, February 2003 (2003-02), pages 86-95, XP009047143 ISSN: 0021-8898 abstract page 87 - page 88, paragraph 1; tables 1-3	1-28,30, 32,34,35
A	JACOBSON R A: "A Monte Carlo method for indexing [crystallography]" ZEITSCHRIFT FUR KRISTALLOGRAPHIE OLDENBOURG GERMANY, vol. 212, no. 10, 1997, pages 689-690, XP009047153 ISSN: 0044-2968 abstract	1-28,30, 32,34,35

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C.(Continuation) DOCUMENTS CONSIDERED TO BE RELEVANT

Category *	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
A	<p>KARIUKI B M ET AL: "A new approach for indexing powder diffraction data based on whole-profile fitting and global optimization using a genetic algorithm" JOURNAL OF SYNCHROTRON RADIATION MUNKSGAARD INTERNATIONAL BOOKSELLERS AND PUBLISHERS FOR INT. UNION CRYSTALLOGR DENMARK, vol. 6, 1 March 1999 (1999-03-01), pages 87-92, XP009047154 ISSN: 0909-0495 page 87 page 89, chapter "4. Search methods"</p>	1-28,30, 32,34,35
A	<p>JIH SHANG HWANG ET AL: "XRAYSCAN: an indexing program considering dense spurious peaks in an optimization method" CHINESE JOURNAL OF PHYSICS PHYS. SOC. REPUBLIC OF CHINA TAIWAN, vol. 34, no. 1, February 1996 (1996-02), pages 47-57, XP002326868 ISSN: 0577-9073 abstract page 48, paragraph 1 page 49, paragraph 3 - page 52, paragraph 1 page 56</p>	1-28,30, 32,34,35
A	<p>R. SHIRLEY: "Overview of powder-indexing program algorithms (history and strengths and weaknesses)" IUCR COMPUT. COMMISS. NEWSLETT., [Online] vol. 2, July 2003 (2003-07), pages 48-54, XP002326869 Retrieved from the Internet: URL: http://www.iucr.org/iucr-top/comm/ccom/newsletters/2003jul/iucrcompcomm_jun2003.pdf [retrieved on 2005-04-27] page 52 - page 53</p>	1-28,30, 32,34,35

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Box II Observations where certain claims were found unsearchable (Continuation of item 2 of first sheet)

This International Search Report has not been established in respect of certain claims under Article 17(2)(a) for the following reasons:

1. ☐ Claims Nos.:
because they relate to subject matter not required to be searched by this Authority, namely:
2. ☐ Claims Nos.:
because they relate to parts of the International Application that do not comply with the prescribed requirements to such an extent that no meaningful International Search can be carried out, specifically:
3. ☐ Claims Nos.:
because they are dependent claims and are not drafted in accordance with the second and third sentences of Rule 6.4(a).

Box III Observations where unity of invention is lacking (Continuation of item 3 of first sheet)

This International Searching Authority found multiple inventions in this international application, as follows:

see additional sheet

1. ☐ As all required additional search fees were timely paid by the applicant, this International Search Report covers all searchable claims.
2. ☐ As all searchable claims could be searched without effort justifying an additional fee, this Authority did not invite payment of any additional fee.
3. ☐ As only some of the required additional search fees were timely paid by the applicant, this International Search Report covers only those claims for which fees were paid, specifically claims Nos.:
4. ☒ No required additional search fees were timely paid by the applicant. Consequently, this International Search Report is restricted to the invention first mentioned in the claims; it is covered by claims Nos.:
1-28, 30, 32, 34, 35,

Remark on Protest

- ☐ The additional search fees were accompanied by the applicant's protest.
- ☐ No protest accompanied the payment of additional search fees.

FURTHER INFORMATION CONTINUED FROM PCT/ISA/ 210

This International Searching Authority found multiple (groups of) inventions in this international application, as follows:

1. claims: 1-28,30,32,34,35

A Monte Carlo algorithm generates potential unit cell solutions iteratively reducing the symmetry and/or increasing the volume of the potential unit cell solutions

2. claims: 29,31,33

A refined method is performed to identify the solution to the unit cell parameters
